Chlorhexidine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 20700 L/kg

Global applicability domain: Outside

Local applicability domain index: 1.68e-01

Confidence level: 6.15e-01

Nearest Neighbors from the Training Set

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Dioctyl phthalate
Measured: 24000
Predicted: 17100

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Bis(2-ethylhexyl) terephthalate
Measured: 14500
Predicted: 12500

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Di(2-ethylhexyl) adipate
Measured: 15500
Predicted: 14400

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Fluvalinate
Measured: 507000
Predicted: 293000

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tau-Fluvalinate
Measured: 507000
Predicted: 284000